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Shuai Shi-jin, Wang Jian-xin, Zhuang Ren-jun and Chen Jun-rui
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ABSTRACT

A mathematical model of the flows in honeycomb monolith was established by an equivalent continuum approach, and the commercial code STAR-CD was utilized to simulate multi-dimensional steady turbulent room airflows in catalytic converters with different configurations. In order to verify the computing model, a pitot tube was used to measure the velocity distribution in the converter. Validations demonstrate that theoretical values agree well with experimental results.

Simulation results show that, the larger the inlet cone angle the more the pressure loss and maldistribution in converters, however, when the angle enlarges enough its effect on flows will be obviously decreased thereafter. An enhanced diffusion header has benefits to the flow characteristics. Compared with the inlet cone angle, the outlet cone angle has little influences on the performance of flows. The spherical shape of the front face of monoliths proposed by authors is capable of improving the flow distribution. The monolith location has no significant effects on the flow quality. In addition, the larger the gap between two monoliths the more uniform the flow distribution for the second monolith but the less for the first. These results offer a practical guide to the optimum design of automotive catalytic converters.

INTRODUCTION

Catalytic converters are being widely used in automobile industry and have already proved for years to be the most effective technical solution to reduce gaseous emissions from S.I. engines. A worldwide demand for environmental protection has enforced more stringent legislation of automotive exhaust emissions. Thus, the requirement for high performance of the catalytic converter tends to be imperative. Not only high conversion efficiency but also a long durability and low flow resistance are essential to automotive catalytic converters. Flow uniformity is critical to ensure a long converter life. Theoretical and experimental studies[1] have shown that poor flow distribution within the monolith could reduce catalyst longevity by locally removing out the precious metal coatings whilst causing deterioration in emissions. Equally important is the fact that high flow resistance of the converter system will limit the peak power of an engine and penalize the vehicle fuel economy. Therefore, it is necessary to investigate the flow characteristics of the converters and then optimize them.

Configurations of the catalytic converter, such as cone geometry, monolith size and position, and so on, are the main factors affecting the flow features of the converter system. In the past, the design of automotive catalytic converters mostly relied on experiments or practices[1,2], and the entire process lasted a long period and also required significant expense. Recently, with the development of the computational capability of the computer, the possibilities and the limitations of a multi-dimensional Computational Fluid Dynamics (CFD) as an industrial design tool have been improved significantly. Thus, simulation method can be used to study the flow characteristics of catalytic converters, such as velocity distributions and pressure losses. Most of the early research studies[3,4], however, have focused on establishing models and simulating the flow fields. Little works has been carried out to investigate the flow characteristics of different converter structures.

The purpose of this study is to use multi-dimensional CFD tools to set up the fluid dynamic mathematical model of catalytic converters and study the structural effects on the flow distribution as well as pressure loss in converters.

THEORETICAL MODELS

GOVERNING EQUATIONS – For general incompressible and compressible steady turbulent fluid flows, the mass and momentum conservation equations are:

$$\frac{\partial}{\partial x_j}(\rho u_j) = 0 \tag{1}$$

$$\frac{\partial}{\partial x_j}(\rho u_j u_i + \tau_{ij}) = -\frac{\partial p}{\partial x_i} + s_i \tag{2}$$

in which s_i is the source term representing monolith resistance (also see equation 9 below) and the stress tensor τ_{ij} for Newtonian turbulent flow is:

$$\tau_{ij} = -\mu\left(s_{ij} + \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right) + \overline{\rho u_i' u_j'} \tag{3}$$

where δ_{ij} is the Kroneker delta and s_{ij} the rate of strain tensor given by:

$$s_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \tag{4}$$

In order to determine the Reynolds stresses and turbulent scalar fluxes a $\kappa - \varepsilon$ turbulence model has been used, comprising differential transport equation for the turbulent kinetic energy κ and its dissipation rate ε. The conventional form of the $\kappa - \varepsilon$ model assumes that the turbulent Reynolds stresses and scalar fluxes are linked to the time-averaged flow properties by:

$$\overline{\rho u_i' u_j'} = -\mu_t s_{ij} + \frac{2}{3}\left(\mu_t \frac{\partial u_k}{\partial x_k} + \rho\kappa\right)\delta_{ij} \tag{5}$$

where the turbulent viscosity μ_t is linked to κ and ε by:

$$\mu_t = \frac{C_\mu \rho \kappa^2}{\varepsilon} \tag{6}$$

The transport equation used to determine the turbulence energy and its dissipation rate are:

$$\frac{\partial}{\partial x_j}\left(\rho\mu_j\kappa - \frac{\mu_t}{\sigma_\kappa}\frac{\partial \kappa}{\partial x_j}\right) = \mu_t s_{ij}\frac{\partial u_i}{\partial x_j} - \rho\varepsilon - \frac{2}{3}\left(\mu_t \frac{\partial u_i}{\partial x_i} + \rho\kappa\right)\frac{\partial u_i}{\partial x_i} \tag{7}$$

$$\frac{\partial}{\partial x_j}\left(\rho\mu_j\varepsilon - \frac{\mu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}\right) = C_{\varepsilon 1}\frac{\varepsilon}{\kappa}\mu_t s_{ij}\frac{\partial u_i}{\partial x_j} - \frac{2}{3}\left(\mu_t \frac{\partial u_i}{\partial x_i} + \rho\kappa\right)\frac{\partial u_i}{\partial x_i}$$
$$- C_{\varepsilon 2}\rho\frac{\varepsilon^2}{\kappa} + C_{\varepsilon 4}\rho\varepsilon\frac{\partial u_i}{\partial x_i} \tag{8}$$

in which C_μ, σ_κ, σ_ε, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$, $C_{\varepsilon 3}$, $C_{\varepsilon 4}$ are further empirical coefficients whose values are given below.

C_μ	σ_κ	σ_ε	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	$C_{\varepsilon 3}$	$C_{\varepsilon 4}$
0.09	1.0	1.22	1.44	1.92	0.0	-0.33

The commercial CFD code STAR-CD[5] was utilized to solve the equations described above. STAR-CD is a three-dimensional elliptic hyperbolic flow simulation code for laminar and turbulent flows in complex geometry. For the steady flow simulation here, the SIMPLE pressure correction algorithm was used and the flow calculation of the converter except for the monolith used the high Reynolds number $\kappa - \varepsilon$ turbulent model, employing the universal law-of-the-wall for the near-wall low-Reynolds number flow region.

MODELING MONOLITHS – Catalyst support can be divided into two main groups, the bead-bed and the honeycomb monolith, based on their shape and structure. Only the honeycomb monoliths extensively used are modeled and analyzed here. A honeycomb monolith consists of a large number of small channels that have the same size and configuration. Although it is conceivable that a monolith could be modeled in its entirety for detailed information, with each individual channel having its fluid dynamic processes simulated, such a model would be prohibitively large. In fact, from an engineering point of view, more attention tends to be paid to the effect of an integrated monolith rather than its microstructure. To avoid using extremely large grids an equivalent continuum approach[6], which views the monolith as a porous medium due to the geometry regularity and small size of the channels, was used to model the monoliths.

The monoliths investigated have an enormous number of quadratic cells and cell density of 400cpsi (cells/in^2). The corresponding brick wall thickness for the monoliths is 0.15mm. The monoliths are modeled as porous media employing a relationship between the pressure and the resistance forces as follows:

$$\frac{\partial p}{\partial x_i} = -K_i u_i \tag{9}$$

$$K_i = \acute{a}_i\left|\vec{V}\right| + \hat{a}_i \tag{10}$$

where x_i are mutually orthogonal directions within the porous region, K_i is the permeability and u_i is the local velocity in direction i. K_i is assumed a quasilinear function of the local velocity magnitude $\left|\vec{V}\right|$. The constants α_i, β_i in the streamwise direction are valued from experimental data along the monolith. High values (10^5) are chosen in other two cross-stream directions because there is no radial mass transfer in the porous media.

MODEL VALIDATION – For any computational model to be of use it must give realistic results. The best way of checking the accuracy of results is to compare them with experimental data. Here, the velocity profiles were chosen for the comparisons.

VELOCITY MEASUREMENT – As the high temperature and dramatic pulsation of exhaust gas are concerned, it is rather difficult to precisely measure the flow properties under real engine conditions. Therefore the test was conducted on a steady flow bench in ambient air. It is reasonable to assume that conclusions obtained from steady room airflows will be suitable for real conditions[5].

Figure 1 shows a schematic of the flow rig. The rig air supply was draw by an air pump. Converters were situated at the inlet of the rig and the air flowed through the converters containing the monolith to the atmosphere. A by-pass valve was provided to allow fine adjustment so as to achieve a constant flow rate and the purpose of the

air tank was to offer an unchanged pressure in the system. A sliding three-hole pitot tube, 3mm internal diameter by 300mm long, was located at the rear of the monolith. Velocity profiles were measured by making a radial traverse. A removable axisymmetric catalytic converter was designed for the convenience of tests as shown in Figure 2. The velocity profiles of different inlet cone angles can be easily measured by removing the inlet cones. The measured velocity profiles can be viewed as the profile inside the monoliths due to its very close distance (10mm) to the monolith.

COMPARISONS BETWEEN PREDICTIONS AND MEASUREMENTS – In order to verify the established model, numerical simulations were performed for the axisymmetric catalytic converters of Figure 1. The studies have focused on axisymmetric system for several reasons. Firstly, these systems are expected to contain many of the important primary flow features associated with more complex geometric configurations--i.e. separated flows with large recirculation. Secondly, the nature of the flow can also be more readily obtained as fewer measurements are needed to characterize the systems (the flow is two-dimensional) and thirdly, the computational resources needed to simulate 2D regions are far less demanding. Finally, it is believed that focusing on simple axisymmetric configurations will aid in the understanding of the relationships between the various controlling parameters and also in the design of more complex systems.

The computational regions of the converters are shown in Figure 3. The number of grid cells used for validations is of the order 185 along the axis by 40 across the radius. The light color of the domains represents the monolith. It is assumed that the velocity distribution of the inlet pipe is uniform. The computational boundaries of the entrance are determined according to measurements as follows: the axial velocity is 53.0m/s, the airflow density is 1.205kg/m^3 and temperature is 293.0K. The inlet κ and ε are calculated under the assumption of 5% turbulence intensity and 1mm mixing length. The outlet boundaries are treated as being fully developed flows—i.e. the velocity gradient is zero.

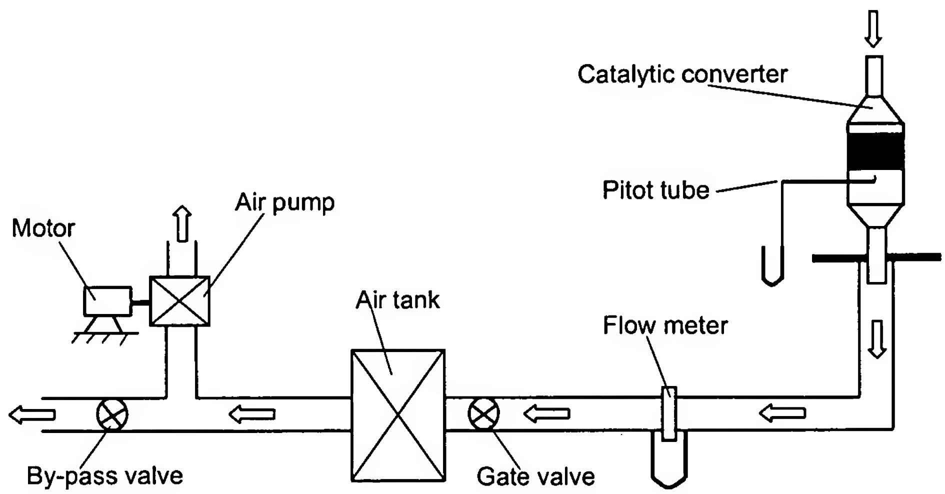


Figure 1. The schematic of the flow rig

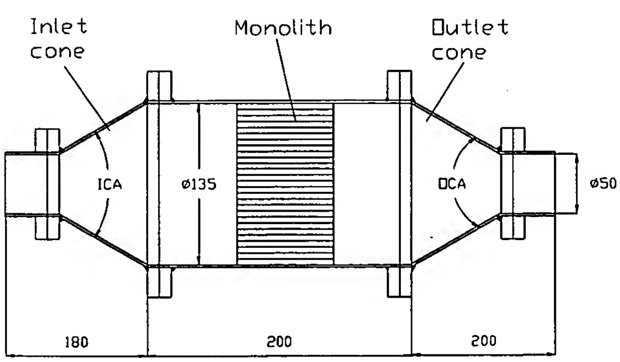
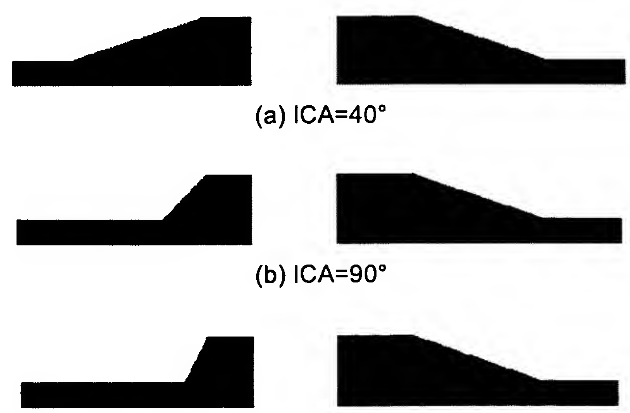


Figure 2. The removable catalytic converter



(a) ICA=40°

(b) ICA=90°

(c) ICA=120°

Figure 3. Computational regions

Figure 4 shows comparisons between the computational velocity distributions and the experimental ones. From the diagram it can be seen that the pattern of the predicted data points is similar to that of the experimental points. Especially, the trend of the flow distribution varying with the ICA was well predicted compared with the one of the tests. This indicates that the established models are feasible and can be used to predict the flow characteristics of the converters with various configurations. There are several possible explanations for the errors between computing and testing. These could be associated with either the turbulence model, numerical inaccuracy or monolith resistance formulation. Of these it would seem that the monolith pressure drop expressions that have been used are a little simplistic. The flow field at the monolith face is clearly very complex featuring flow with high curvature. But the accuracy of the model is high enough for the comparative studies of the catalytic converters.

RESULTS AND DISCUSSION

On the basis of the validation of the model, various structures and configurations of the converters, including different inlet and outlet cone angles, different shapes, sizes and positions of the monoliths and the like, were chosen to be simulated and analyzed.

INFLUENCE OF INLET CONES – To see the influence of the inlet cone angle (ICA) on flow distribution and pressure loss, three cases just the same as those in the validation were analyzed. In all cases, the structural parameters except for ICA and computational conditions are identical. Figure 5 shows the influence of ICA on the flow features, where Figure 5(a) is the axial velocity profiles over the radial direction at the rear of monoliths and Figure 5(b) is the total pressure distribution along the axis of the converters at the center of cross section. The total pressure losses of the converter could be approximately obtained by subtracting the pressure value at the outlet from the one at the inlet according to Figure 5(b). It can be seen from the figure that the ICA has an important effect on the flow characteristics. The flow maldistributions and pressure losses in the case of 90°and 120° are much larger than those in the case of 40°. However, the velocity profiles and pressure drops of 90°and 120°cases are similar and have no significant differences. An explanation for the different variations is given below. As the ICA increase, the flow is detached from the wall of the cone pipe to form a recirculation, as shown in Figure 6, and cause a partial pressure loss. Thus, the larger the ICA, the less the flow uniformity and the more the pressure loss. But when ICA enlarges to a value, a jet flow is formed. Thus, the flow separation is not sensitive to the contour of the inlet cone and the influence of the ICA on the flow features becomes weak.

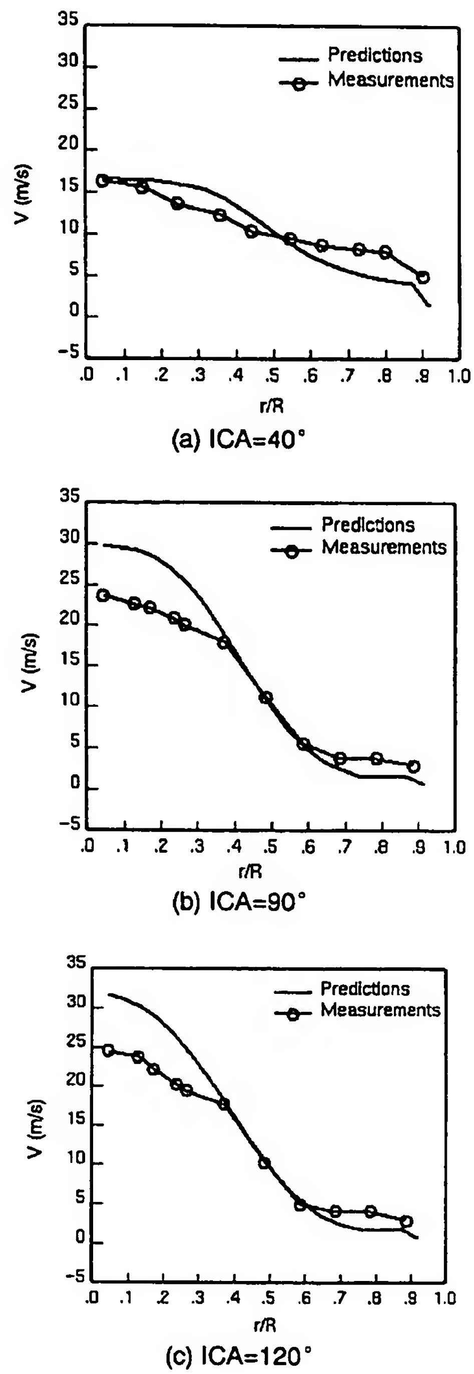
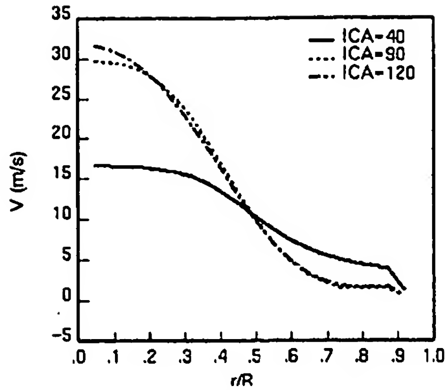
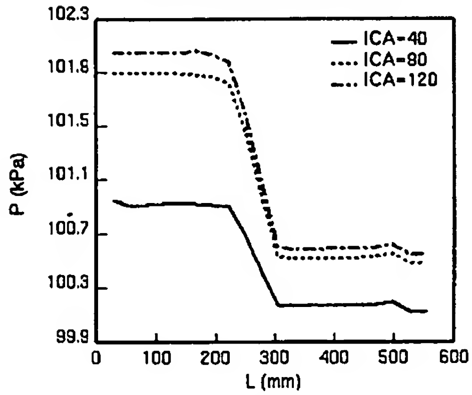


Figure 4. Comparisons of predictions and measurements



(a) Axial velocity profile



(b) Pressure distribution

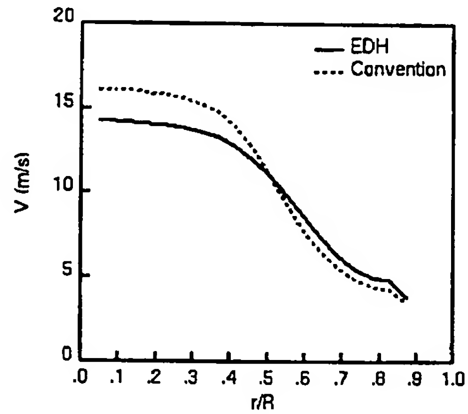
Figure 5. Influence of ICA


(a) Conventional inlet cone

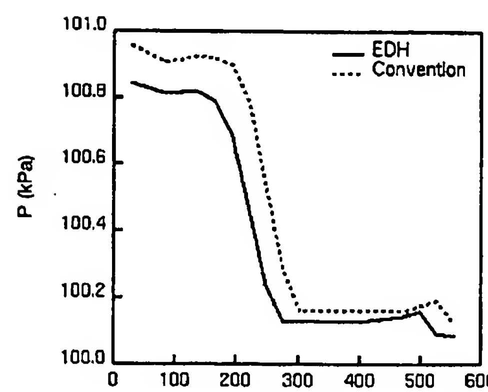

(b) EDH

Figure 7. Computational regions

In order to investigate the influence of the inlet cone on the flow an enhanced diffusion header (EDH) was designed as shown in Figure 7(b). This combines a short, shallow-angle diffuser with a more abrupt expansion to the monolith cross section. The main purpose of the EDH originally developed by Wendland[7], based on the principle of gas fluid dynamics, was to reduce the pressure loss of the inlet diffuser, which was verified through a series of tests. The previous work, however, focused on the experiment and did not run any numerical simulations on the flows in EDH. Therefore, the flow mechanism of EDH can not be well understood. The EDH of Figure 7(b) is characterized by a 12°ICA shallow diffuser and a sudden expansion from the distance of 25mm to the front monolith. A conventional inlet diffuser, shown as in Figure 7(a), was simultaneously analyzed with the EDH for comparing. The structure except for the inlet cone and the computational conditions of the two converters were identical. Figure 8 shows the comparisons of the flow profile and pressure distribution between EDH and conventional inlet cone. Figure 9 is the amplified inlet velocity vectors. From Figure 8 it is obviously seen that EDH is capable of improving the flow distribution and simultaneously reducing the pressure loss. The reason for the benefits of EDH is that a small ICA causes no separations from the wall of the transition diffuser and a narrow abrupt space limits the recirculation occurring in front of the monolith (see Figure 9).



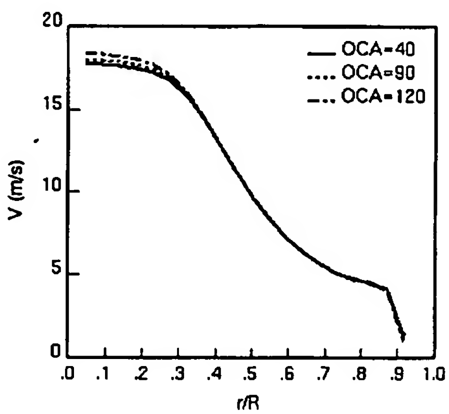
(a) Axial velocity profile



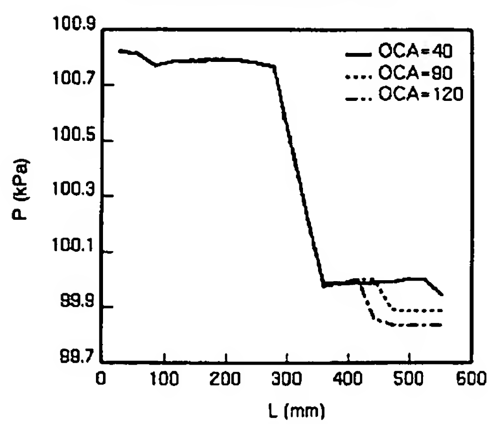
(b) Pressure distribution

Figure 8. Influence of EDH

INFLUENCE OF OUTLET CONES – The influence of the outlet cone angle (OCA) on the flow quality of the catalytic converter is shown in Figure 10. The varying OCA is 40°, 90°and 120° respectively and the ICA is 40°. Figure 11 shows amplified velocity vectors of the outlet cone. From Figure 10(a) we can see that the OCA has little influence on the flow distribution in the monoliths. But Figure 10(b) indicates that the OCA has a little effect on the pressure loss of the converter. The pressure losses caused by OCA are located at the interface between the outlet cone and the outlet pipe. It can also be seen that the 40°OCA almost has no loss at the interface, but as the OCA enlarges the partial pressure losses will be increase. Compared with the pressure losses caused by the inlet cone, however, the losses by the outlet cone are much smaller. Combining Figure 11 and Figure 6 we can clearly observe that the vortexes in inlet cones are much bigger than those in outlet cones, which occur only near the interface between the outlet cone and the outlet pipe.



(a) Axial velocity profile



(b) Pressure distribution

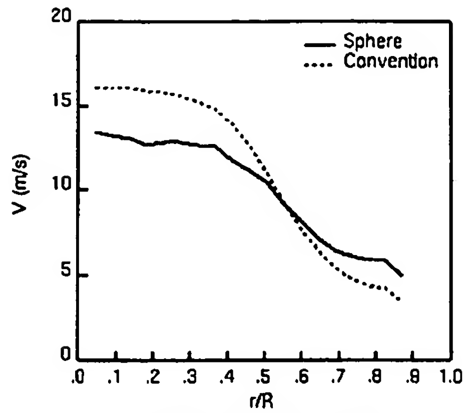
Figure 10. Influence of OCA

INFLUENCE OF MONOLITHS

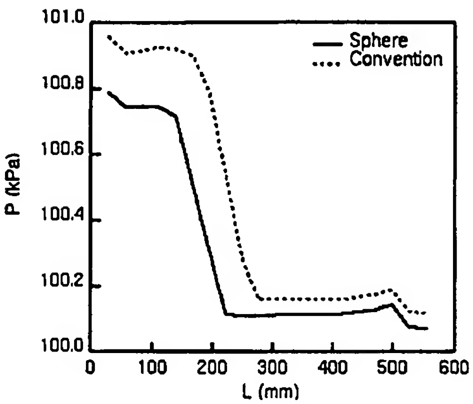
<u>Front face shape</u> – In order to explore the influence of the front face shape of the monolith on the flows, a spherical monolith, as shown in Figure 12, was chosen as a research object. The idea of the spherical shape of the monolith was first proposed by authors in an experimental study on the catalytic converters[8]. It has been found that the spherical shape can lead a more uniformity of the flow distribution. Here, effects of the spherical monolith observed in the test are expected to be explained by a detailed simulation. The study on the spherical monolith is also conducted with a conventional flat monolith, as shown in Figure 7(a), which has the same volume as the spherical. Figure 13 shows the comparison of the flow characteristics between the two monoliths. The amplified velocity vector is shown in Figure 14. Figure 13(a) shows that the spherical shape can indeed improve the flow distribution. The main reason for the improvement is that the spherical monolith can be partially embedded into the inlet cone, thus reducing the flow recirculation region in the inlet cone as shown in Figure 14. In addition, the airflow in the center will flow toward the periphery due to the spherical configuration of the monolith, causing flow distribution more uniform. The spherical shape acts as a deflector in a sense. From Figure 13(b) we can know that the pressure loss of the spherical converter is a little smaller than that of the conventional, which results from a more uniform flow distribution of the spherical shape. The computational results are consistent with the tests.

Figure 12. Computational region of the spherical monolith

<u>Position</u> – Two fixed positions of a single monolith—i.e. the top as shown in Figure 7(a) and the middle as shown in Figure 3(a)--were run to study the influence of the monolith location on the flow. Figure 15 shows the influence of the monolith position on the flows. It can be observed that the flow distribution and pressure loss in the monolith at the top of the canister are very similar to those at the middle, which means the position of the monolith has no large influence on the flow features in the converters. This is because the gas flow has been fully diffused after passing through the inlet cone header.



(a) Axial velocity profile

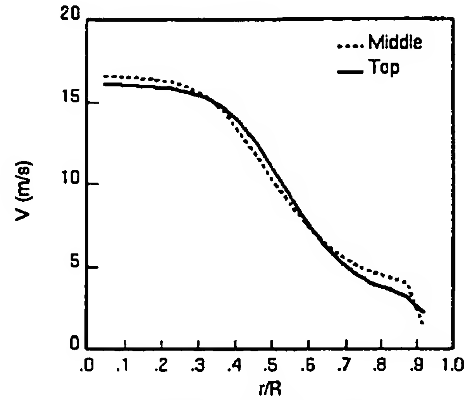


(b) Pressure distribution

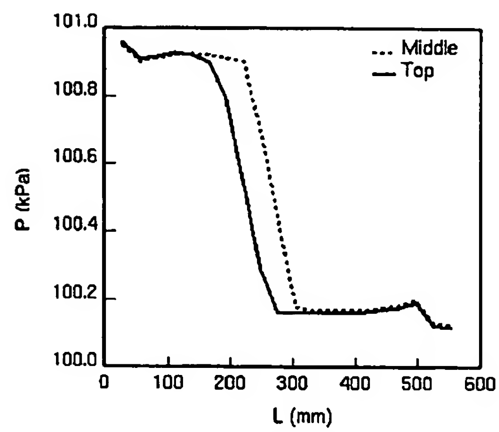
Figure 13. Influence of the spherical monolith

In this case, even though the location of the monolith changes a lot the flow characteristics of the monolith have no significant variations.

Length – The catalytic converters with a single-monolith (see Figure 7(a)) and a double-monolith (see Figure 17(a)) were simulated to study the influence of the monolith length on the flows in the converters, as shown in Figure 16. It can be obtained from the Figure that the double-monolith has a better velocity distribution and higher pressure loss than the single-monolith. This is because the flow resistance of the monolith is proportional to its length. Therefore, the double-monolith has a higher flow resistance than the single-monolith, leading a full diffusion in front of the monolith and resulting in a more uniform velocity distribution in the monolith. However, it is not wise to improve the flow distribution by increasing the flow resistance, because this will also lead to a penalty of engine performances. How to balance the pressure loss and flow distribution should be carefully considered when designing a converter.

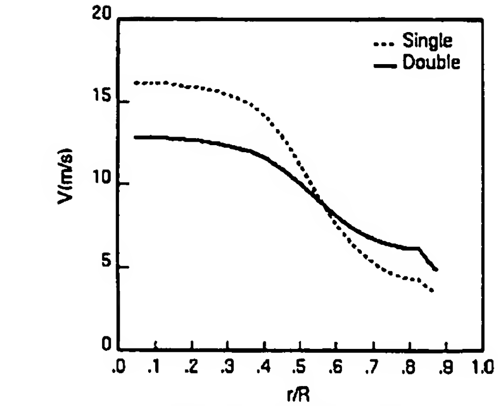


(a) Axial velocity profile

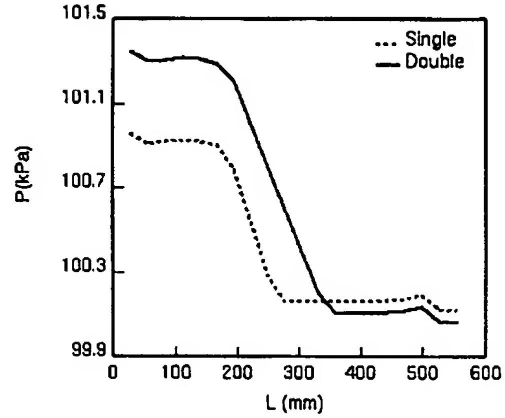


(b) Pressure distribution

Figure 15. Influence of the monolith position



(a) Axial velocity profile



(b) Pressure distribution

Figure 16. Influence of the length

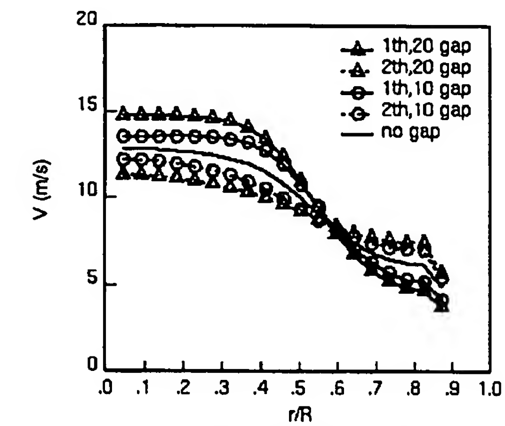
Gap between monoliths – The influence of the gap between monoliths on flow distribution and pressure loss was investigated by changing the distance between monoliths with three cases as shown in Figure 17. Figure 18 illustrates the comparison of the velocity profile over the monoliths and the total pressure distribution along the axis with different gaps. In Figure 18(a) it is shown that the flow distribution in the first and second monolith are very different. The change of the distribution takes place in the space between the monoliths. With increasing distance between monoliths, the difference in the velocity of the inner and outer regions increases for the first monolith while decreasing for the second monolith. This means that the larger the gap between monoliths, the less uniform the distribution with the first monolith but the more uniform the distribution in the second monolith. With no gap between the monoliths the velocity distribution is similar inside both monoliths. From Figure 18(b) we can find that the gap between the monoliths almost has no significant impact on the pressure drop. In practice, the gap between the monoliths is unavoidable, the inconsistency of flow distribution between the first monolith and second monolith should be fully considered. In general, from the fluid dynamics point of view a small gap is expected when designing a double-monolith catalytic converter.

(a) no gap

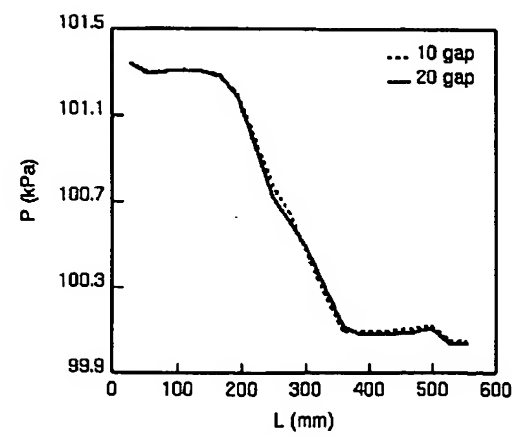
(b) gap=10

(c) gap=20

Figure 17. Computational regions



(a) Axial velocity profile



(b) Pressure distribution

Figure 18. Influence of the gap

CONCLUSIONS

From this study of the flows in the automotive catalytic converters with various configurations it is conclude that:

- The equivalent continuum approach, which viewed the honeycomb monolith as a medium, was well employed to build the fluid dynamic model of the monolith. The CFD commercial code STAR-CD was successfully used to simulate the steady room airflows in the entire catalytic converters.
- Validation of the model illustrates that the computational results show good agreement with the experiments, which means modelling the converters can be utilized to predict the flow features in the converters with different configurations.
- The inlet cone angle (ICA) has a significant effect on the flow characteristics of the converters. The larger the ICA, the higher the flow maldistribution and pressure loss in the converters.
- EDH can apparently improve the velocity uniformity in the monoliths and also reduce the converter pressure loss.
- Compared with inlet cone, the outlet cone has little influence on the flows.
- The spherical face shape used for the monolith is a hopeful measure to improve the flow distribution in the monolith.
- The flow quality is not sensitive to the position of the monolith in the canister. But the longer the monolith the more uniform the flow distribution and the higher the flow resistance in the converter.
- The gap between the monoliths can improve the flow distribution of the second monolith and simultaneously cause a maldistribution in the first monolith. But the gap has no important impact on the pressure loss.
- Combined with experimentation, CFD is an efficient and reliable approach for optimizing the structure and configuration of the catalytic converters.

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NOMENCLATURE

ρ : the fluid density;

p : the static pressure;

u_i, u_j : the velocity component in i and j direction;

s_i : the source term;

τ_{ij} : the stress tensor;

s_{ij} : the rate of strain tensor;

δ_{ij} : the Kroneker delta;

μ : the laminar viscosity;

μ_t : the turbulent viscosity;

$\overline{\rho u_i' u_j'}$: the turbulent Reynold stress;

κ : the turbulent kinetic energy;

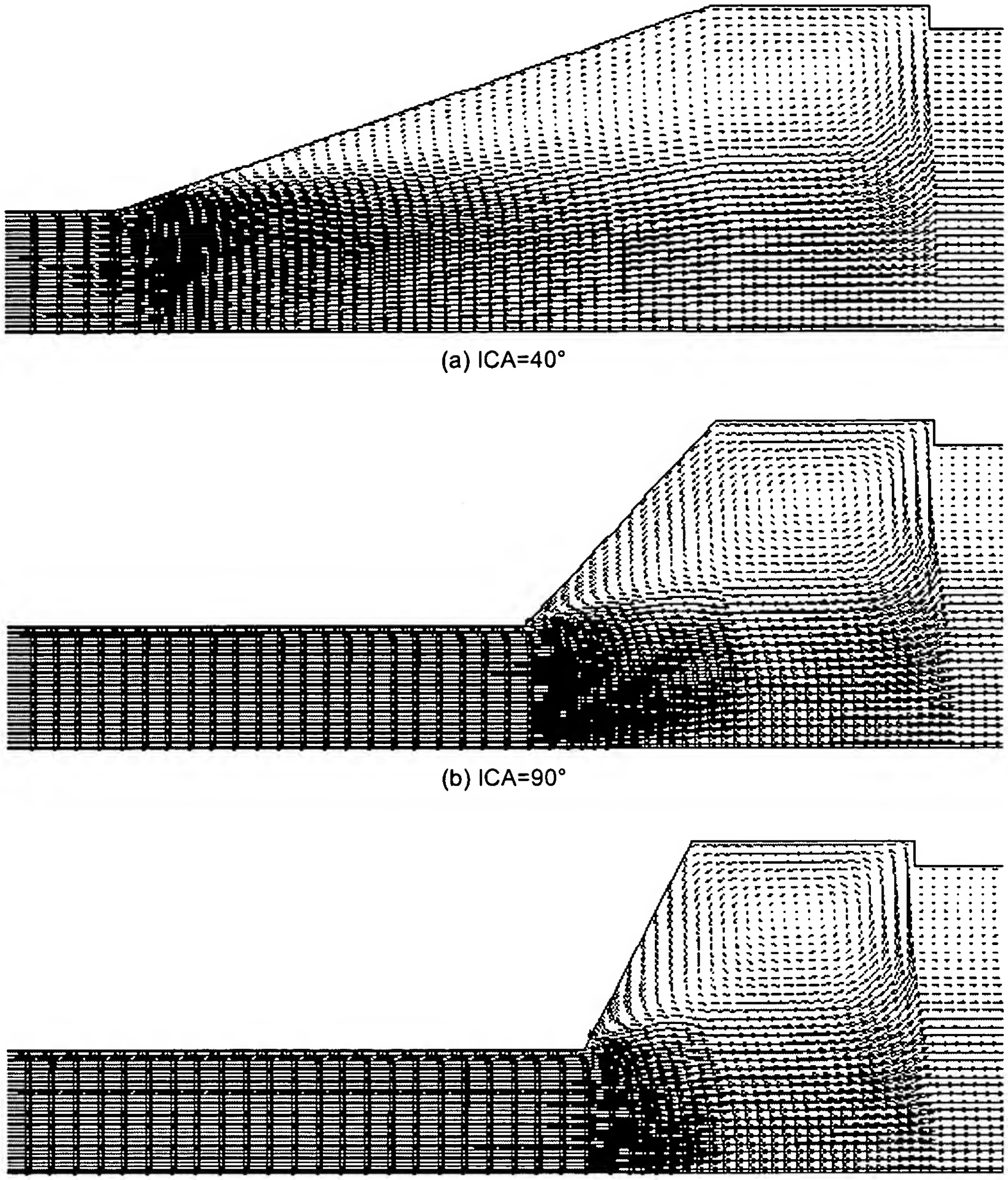
ε : the turbulent dissipation rate;

C_μ, σ_κ, σ_ε, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$, $C_{\varepsilon 3}$, $C_{\varepsilon 4}$: empirical coeffients for the turbulent model;

K_i : the permeability of the monolith;

$|\vec{V}|$: the local velocity magnitude in monoliths;

α_i, β_i : constants in the streamwise direction.

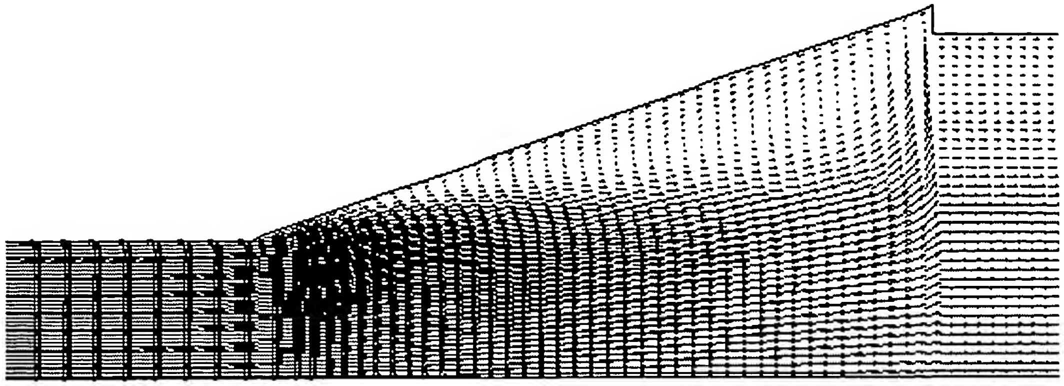


(a) ICA=40°

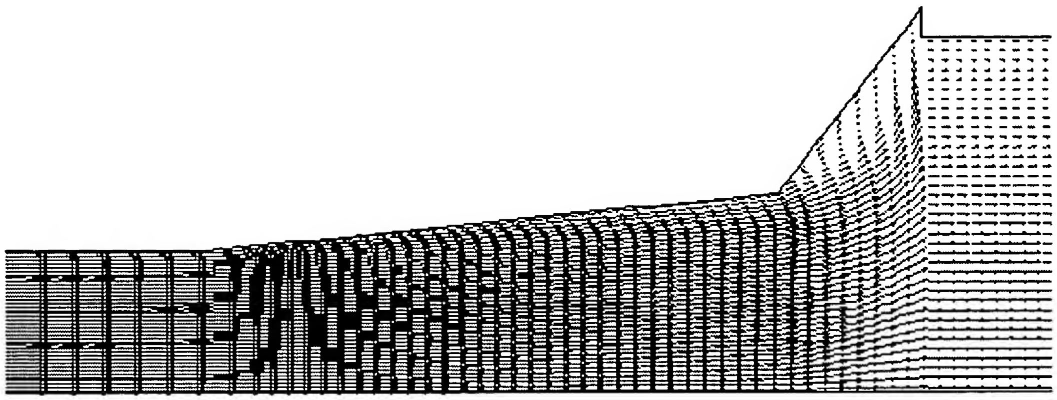
(b) ICA=90°

(c) ICA=120°

Figure 6. Amplified velocity vectors of the inlet cone



(a) Conventional inlet cone



(b) EDH

Figure 9. Amplified velocity vectors of conventional inlet cone and EDH

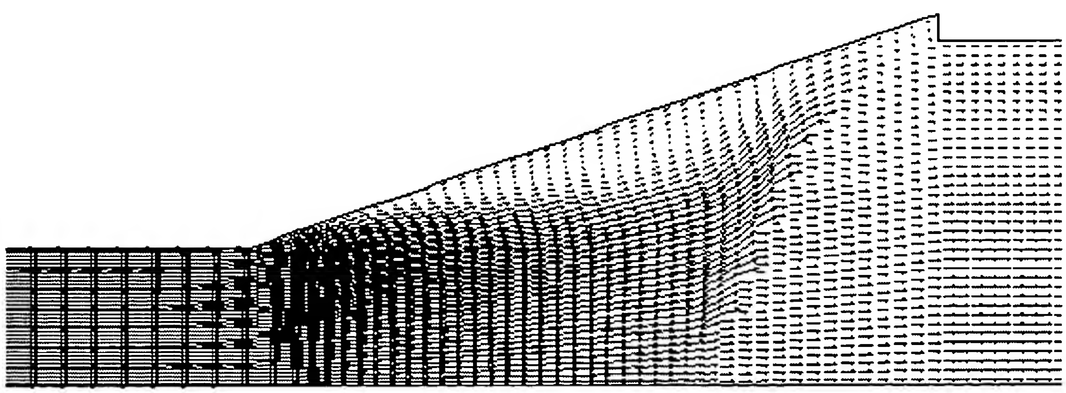
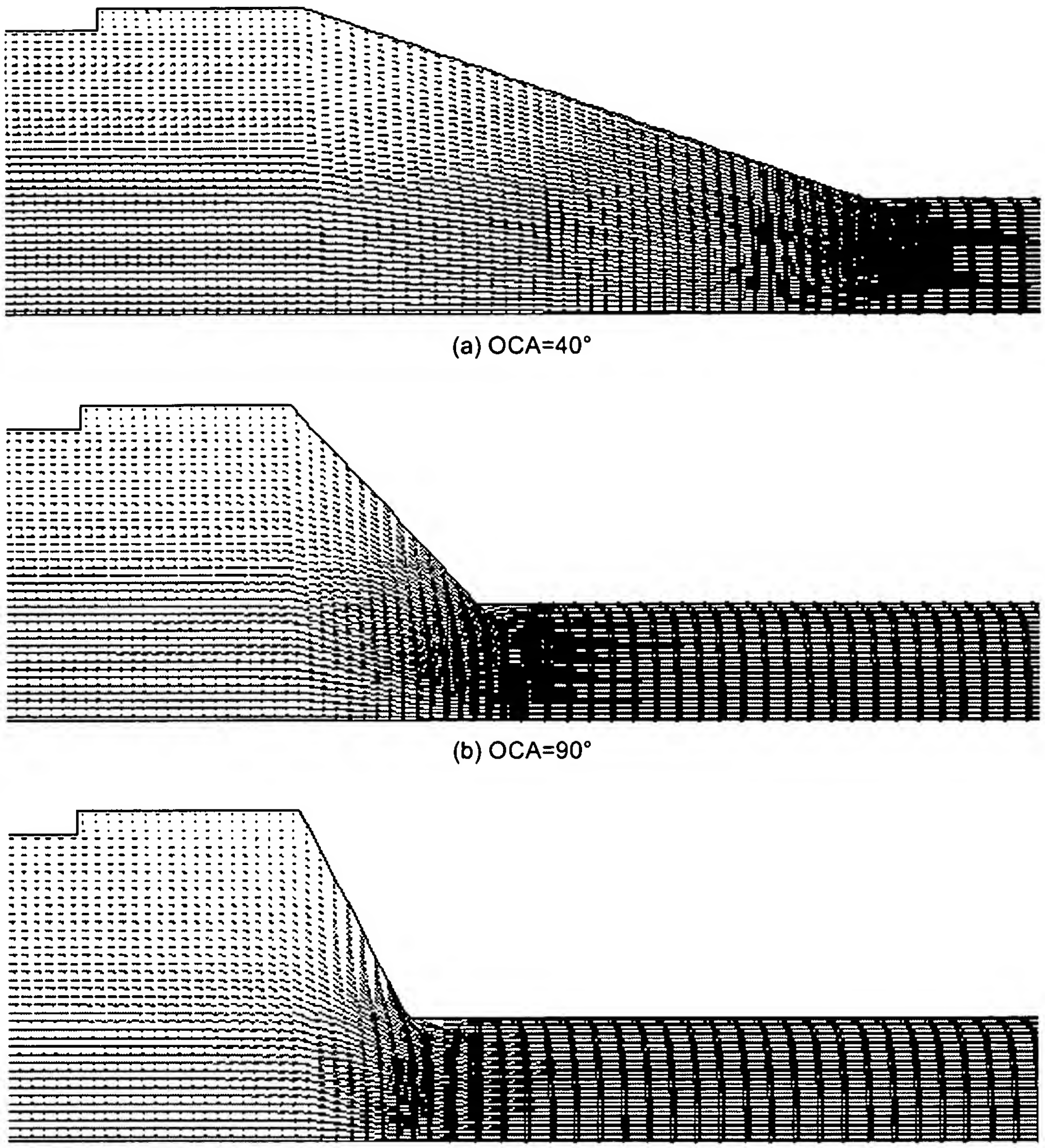


Figure 14. Amplified velocity vector of the spherical monolith



(a) OCA=40°

(b) OCA=90°

(c) OCA=120°

Figure 11. Amplified velocity vectors of the outlet cone